

ID: Plenary III

Title: COMPUTATIONAL PHYSICS OF BIOMOLECULES

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Biological macromolecules are nature's most finely tuned materials. We discuss the properties of biomolecules as seen by theory and computer simulation. We examine the protein glass transition, anomalous internal subdiffusion, binding phenomena and protein folding. Energy landscape approaches to describing kinetically metastable states of proteins are described. Simulation approaches to understanding biomolecular machines are outlined, with an example from muscle contraction. The scaling of molecular dynamics simulation to ~100k cores on the ORNL Jaguar XT5 supercomputer is described. Applications of simulation methods to biofuel research are given.